AD-A157 038 THERMODYNAMICS OF POLYMER-SUPERCRITICAL SOLVENT MIXTURES(U) JOHNS HOPKINS UNIV BALTIMORE MD DEPT OF CHEMICAL ENGINEERING M A MCHUGH 03 JUL 85 1/1

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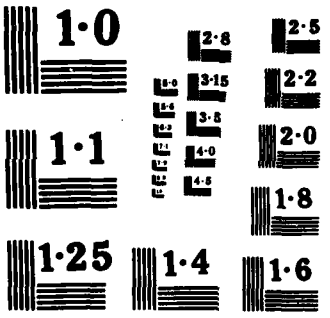
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OFFICE OF NAVAL RESEARCH

Contract N00014-83-K-0613

Task No. NR 625-841

July 1983 - June 1985

Final Technical Report

July 3, 1985

"Thermodynamics of Polymer-Supercritical Solvent Mixtures"

by

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Project Abstract

The objectives of this research are to experimentally investigate the high pressure fluid phase behavior of polymer solutions and to characterize the resultant phase behavior using contemporary polymer solution theories. The polymer solutions of interest are of three types: (1) a binary mixture of polymer and organic solvent, (2) a binary mixture of polymer and supercritical fluid (SCF) solvent, and (3) a ternary mixture of polymer, organic solvent, and SCF solvent.

There are three goals of the experimental phase of this project. The first goal is to determine the effect of high pressure on the lower critical solution temperature (LCST) of the polymer - organic solvent mixture at conditions close to the critical point of the organic solvent. The second goal is to study the phase behavior of polymer - SCF solvent mixtures. The final experimental goal is to study the high pressure phase behavior of ternary mixtures consisting of a polymer, an organic solvent, and an SCF solvent.

Significant Results

Within the duration of this contract the equipment needed to realize experimental goals of this proposal was built. The phase behavior of two model ternary mixtures were studied. These two systems were polystyrene-toluene-SCF carbon dioxide and polystyrene-toluene-SCF ethane. Various concentrations of the SCF solvents were used in determing several Pressure-Temperature projections of the phase border curves for these mixtures. The SCF had the effect of shifting the location of the phase border curves to lower temperatures. More details on the actual phase behavior are presented in Technical Report 2.

Modelling of polymer phase behavior using a modified Patterson's corresponding states theory is presented in Technical Report 1 and Technical Report 2. The phase behavior is represented moderately well with this theory.

Summary of Future Plans

Further phase behavior studies will be carried out on the polystyrene-toluene-SCF ethane and polystyrene-toluene-SCF carbon dioxide systems. Compositional data will be determined, in the two phase

region, for these systems, indicating the efficiency of the separation. The molecular weight distribution of the polymer in the two phases will also be determined. This will determine the extent of fractionation of the polymer, that is ocurring between the two phases. Finally the corresponding states theory of Patterson will be modified to take into account the polydispersity of the polymer. This will enable the theory to be used to predict the fractionation of the polymer. Other modifications will be carried out in an attempt to improve the model.

Personnel Working on the Project

The personnel working on this project from July 1983 to June 1985 include:

Alan K. McClellan

B.S. Chemical Engineering, Imperial College, London, England

M.S. Chemical Engineering, Notre Dame University, Notre Dame, IN

Alan is a Ph.D. candidate.

Time on the project : July 1983 - June 1985.

Even G Bauman

B.E.S. Chemical Engineering, Johns Hopkins University, Baltimore, MD

M.S. Chemical Engineering, University of Notre Dame, Notre Dame, IN

Time on the project : September 1983 - October 1984.

An undergraduate Steve Watson assisted on the experiments from September 1984 - May 1985.

Technical Reports and Journal Articles

Contract N00014-83-K-0613

Task No. NR 625-841

Technical Report No. 1

10/30/84

"Separarting Polymer Solutions Using High Pressure LCST Phenomena", by Alan K. McClellan and Mark A. McHugh

In press, Journal of Polymer Engineering and Science, 1985.

Contract N00014-83-K-0613

Task No. NR 625-841

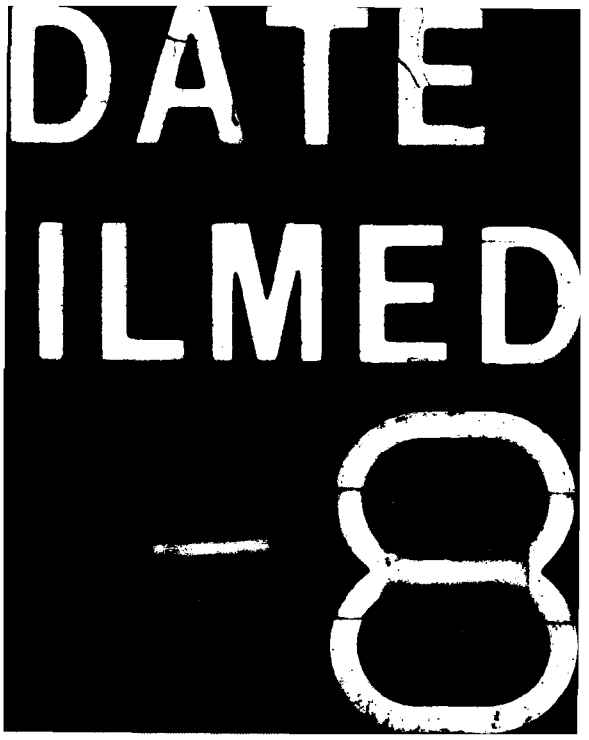
Technical Report No. 2

4/10/85

"Polymer Solution-Supercritical Fluid Phase Behavior",

by Alan K. McClellan, Evan G Baumen, and Mark A. McHugh

In press, in Supercritical Fluid Technology, Penninger, J.M.L., Radosz, M., McHugh, M.A., and Krukonis, V., Eds., Elsevier Science Publishers, Netherlands, 1985.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